

Contents

- Open Data File that contains analysis report from CHN instrument
- Assign variable names to data columns
- Indexing
- Instrument signals for each element
- Run calibration curves
- Carbon -- Amount of C in mg for K1 (acetanilide) runs
- Plot Carbon Calibration curve
- C regression statistics
- Nitrogen -- Amount of C in mg for K1 runs
- Linear regression of std_N as a f(x) of NR signal
- N regression statistics
- C and N (in mg) in filter samples and filter blanks
- Blank corrections
- Nitrogen
- Analysis Report with filter blank-corrected results for C & N
- QA/QC

```
%  
%Script to read and process runs from the Perkin Elmer CHN 2400  
% element analyzer. The code calculates C & N content on sample  
% filter replicates  
clear  
close all  
  
% Data info  
  
cruise = 'P03'; %enter here cruise or campaign code  
  
batch = 'III';  
  
airs=7; % Number of air blanks run at the begining of run prep
```

Open Data File that contains analysis report from CHN instrument

```
filename = uigetfile('/Users/joaquin/Documents/CVO/Lab stuff/POC/Runs/*.csv',...  
    'Select CHN run file');  
  
fid = fopen(filename);  
  
C_text = textscan(fid, '%s', 11, 'delimiter', ',' );  
  
C_data = textscan(fid, '%s %f %f %s %f %f %f %f %f %f %f', 'delimiter', ',' );  
  
fclose(fid);
```

Assign variable names to data columns

```
names = C_text{1};

id      = C_data{1};
seq     = C_data{2};
weight  = C_data{3};
time    = C_data{4};
carbon  = C_data{5};
hydrogen = C_data{6};
nitrogen = C_data{7};
zr      = C_data{8};
cr      = C_data{9};
hr      = C_data{10};
nr      = C_data{11};
```

Indexing

```
%Find index for each type of run (i.e., K factors, blanks, ...
%    ref material, filter blanks, sample, etc

K1s    = find((strcmp(id,'K1') == 1));           %index of K factors calibration ...
                                                %runs (i.e., acetanilide cal runs)
blanks = find((strcmp(id,'BLANK') == 1));         %index of analytical cal blanks
f_blk = find((strcmp(id,'TEST') == 1));           %index of filter, "method blanks"
buff   = find((strcmp(id,'BUFF') == 1));           %index of Buffalo River sediment runs
ace    = find((strcmp(id,'ACE') == 1));            %index of acetanilide check standards

cals   = [K1s; blanks];                           %index of cal runs
stds   = [buff; ace];                            %index of standard & check runs

length_run = size(id,1);
run       = 1:length_run;

samples      = setdiff(run, [cals; stds; f_blk]); %index of sample runs
non_cal      = setdiff(run, cals);
```

Instrument signals for each element

```
%Carbon                      % Carbon signal [i.e., C read (cr)-N read (nr)]
%Blanks
CBs=cr(blanks)-nr(blanks); % C blanks

CB=mean(CBs(1:end-airs));   % Mean C blanks, except air blanks
                            % (run report runs chron. bottom to top)

CS = (cr - nr)-CB;        % Carbon signals (i.e. C read - N read)

%Nitrogen                     % Nitrogen signal [i.e., N read (nr)-zero read (zr)]
%Blanks
```

```

NBs=nr(blanks)-zr(blanks); % N blanks

NB=mean(NBs(1:end-air)); % Mean N blanks, except air blanks

NS = (nr - zr)-NB; % Nitrogen signals (i.e. N read - zero read)

```

Run calibration curves

Carbon -- Amount of C in mg for K1 (acetanilide) runs

```

K1_C    = (71.09/100).*weight(K1s); %mg C per K1 run

% Linear regression of K1_C as a f(x) of C signal, CS.

x = CS(K1s);
y = K1_C;

xx = union(0,x);

C_model = polyfit(x,y,1); %Ace std C vs C signal linear fit
z = polyval(C_model,xx);

```

Plot Carbon Calibration curve

```

f = figure('Position',[2000 1000 550 550]);
subplot(2,1,1);
plot(x,K1_C,'o')
grid on
hold on

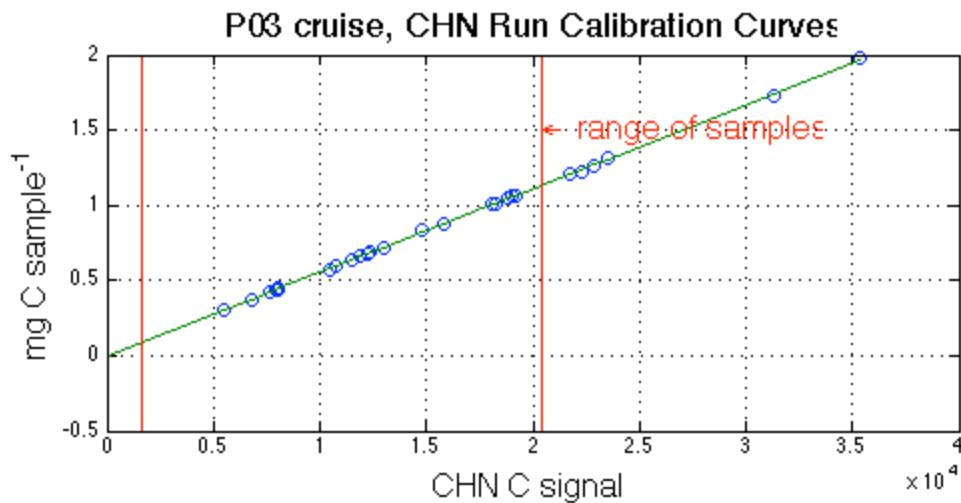
title([cruise ' cruise, CHN Run Calibration Curves'], 'FontSize', 17);

plot(x,y,'o', xx,z , '-')
ylabel('mg C sample^{-1}', 'FontSize',16)
xlabel('CHN C signal', 'FontSize', 16)

aa=get(gca,'xlim');
bb=get(gca,'ylim');

vline([max(CS(samples)), min(CS(samples))], 'r') %vert red lines
%enclose sample
%range
text(max(CS(samples)),bb(2)*.75,' \leftarrow range of samples',...
'color','r','FontSize', 16)

```



C regression statistics

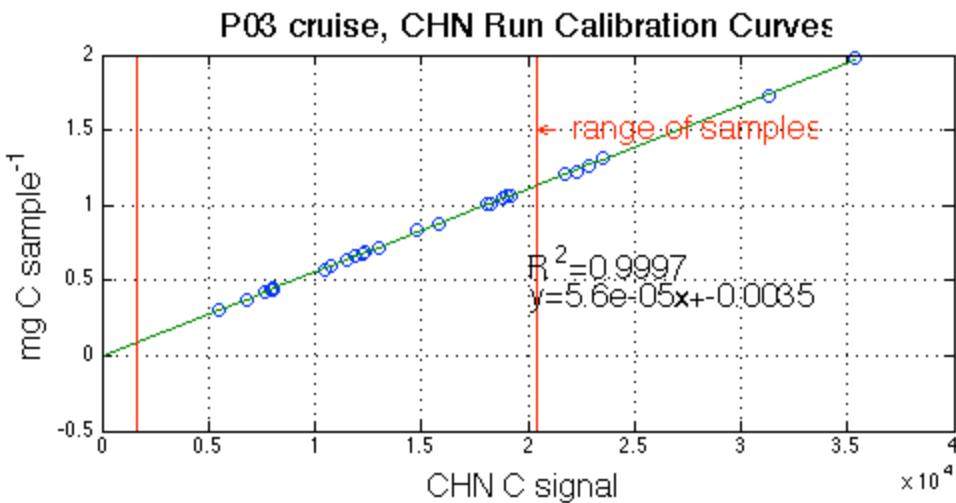
```

X =[ones(size(x,1),1) x];
[b,bint,r,rint,stats] = regress(y,X);

% Display R^2 & regression eq on cal curve plot
text(aa(2)*.5,bb(2)*.3,['R^2=' num2str(stats(1),4)],'fontsize',16)
text(aa(2)*.5,bb(2)*.2,['y=' num2str(b(2),2) 'x+' num2str(b(1),2)],'fontsize',16)

hold off

```



Nitrogen -- Amount of C in mg for K1 runs

```
K1_N = (10.36/100).*weight(K1s); %mg N per K1 run

% Linear regression of K1_N as a f(x) of N signal, NS.

x = NS(K1s);
y = K1_N;
```

Linear regression of std_N as a f(x) of NR signal

```
nx = NS(K1s);
ny = K1_N;

nxx = union(0,nx);

N_model = polyfit(nx,ny,1);
nz = polyval(N_model,nxx);
```

```

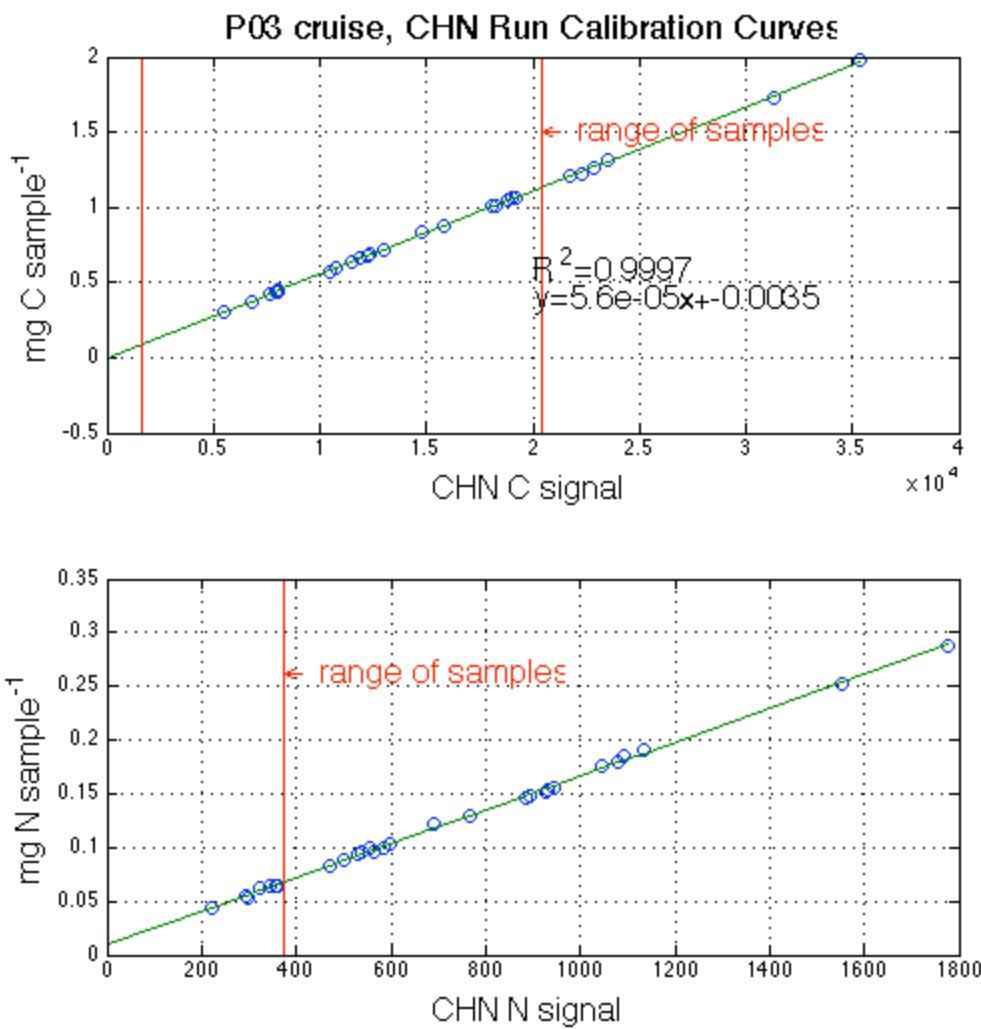
subplot(2,1,2);
plot(nx,K1_N, 'o')
grid on
hold on

plot(nx,ny, 'o', nxx,nz ,'-')
ylabel('mg N sample^{-1}', 'FontSize', 16)
xlabel('CHN N signal', 'FontSize', 16)

aa=get(gca,'xlim');
bb=get(gca,'ylim');

vline([max(NS(samples)), min(NS(samples))], 'r') %vert red lines
%enclose sample
%range
text(max(NS(samples)),bb(2)*.75, '\leftarrow range of samples',...
'color','r','FontSize', 16)

```



N regression statistics

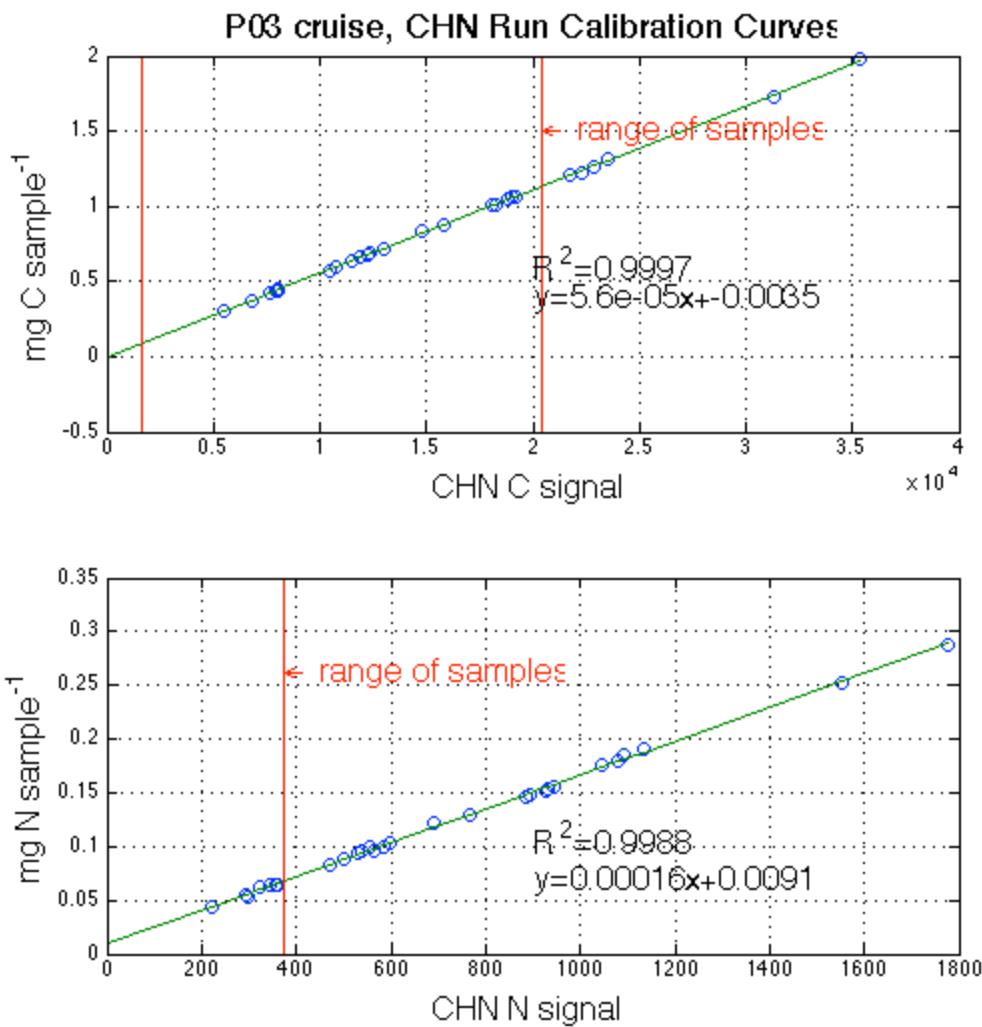
```

NX =[ones(size(x,1),1) nx];
[n_b,n_bint,n_r,n_rint,n_stats] = regress(ny,NX);

% Display R^2 & regression eq on cal curve plot
text(aa(2)*.5,bb(2)*.3,['R^2=' num2str(n_stats(1),4)],'fontsize',16)
text(aa(2)*.5,bb(2)*.2,['y=' num2str(n_b(2),2) 'x+' num2str(n_b(1),2)],'fontsize',16)

hold off

```



C and N (in mg) in filter samples and filter blanks

```

mgC = polyval(C_model,CS(samples)); %C in samples, mg, not corrected for filter blank
mgC_b = polyval(C_model,CS(f_blk)); %C in filter blank

```

Blank corrections

```

if(mean(mgC_b)>0) % C filter blank correction if > 0

```

```

        % if blank < 0, left uncorrected
corr_C = mgC-mean(mgC_b); disp('C filter blanks > 0, correction applied')
else
    corr_C = mgC; disp('C filter blanks < 0, no correction applied')
end

```

C filter blanks > 0, correction applied

Nitrogen

```

mgN = polyval(N_model,NS(samples));          % N in samples, mg, not corrected for filter blank
mgN_b = polyval(N_model,NS(f_blk)); % N in filter blanks

if(mean(mgN_b)>0)                         % N filter blank correction if > 0
corr_N = mgN-mean(mgN_b); disp('N filter blanks > 0, correction applied')
else
    corr_N = mgN; disp('N filter blanks < 0, no correction applied')
end
%
```

N filter blanks > 0, correction applied

Analysis Report with filter blank-corrected results for C & N

```

rep = [str2double(id(samples)),corr_C, corr_N];

f = figure('Position',[1370 85 320 450]);
cnames = {'Sample_ID','C, mg','N, mg'};
t = uitable;
set(t,'Data',rep,'ColumnName',cnames,'Position',[10 0 300 450])

dlmwrite ([cruise '_CHN_run_report_' batch], rep) % Writes report file with sample ID...
% mg C and mg N for each
% sample run

```

	Sample_ID	C, mg	N, mg
1	54	0.1628	0.0237
2	48	0.2845	0.0435
3	42	0.1423	0.0169
4	35	0.4836	0.0333
5	95	0.1188	0.0151
6	73	0.0820	0.0108
7	49	0.2776	0.0421
8	80	1.0465	0.0626
9	83	0.1457	0.0203
10	33	0.1513	0.0275
11	70	0.0877	0.0133
12	75	0.1558	0.0207
13	52	0.1867	0.0313
14	98	0.0664	0.0083
15	19	0.1679	0.0303
16	79	0.0934	0.0143
17	55	0.1850	0.0232
18	74	0.1377	0.0195
19	21	0.1113	0.0125
20	69	0.2650	0.0313
21	45	0.2714	0.0322
22	47	0.3300	0.0509
23	9	0.1934	0.0195
24	65	0.3552	0.0225
25	15	0.0686	0.0113



QA/QC

```
% Carbon percent error based on Buffalo River runs
%NIST certified C % content in Buff R. sed. is 3.51%

%Buffalo River Sediment Ref stds
mgC_buff=polyval(C_model,CS(buff)); % measured C in Buff stds

mgC_buff_t=.0351*weight(buff); % expected C in Buff stds

%ACE check stds
mgC_ace=polyval(C_model,CS(ace)); % measured C in ACE chk stds

mgC_ace_t=.7109*weight(ace); % expected C in ACE chk stds

figure('Position',[2000 100 350 650]);

subplot(2,1,1)

plot(mgC_buff_t,mgC_buff,'o')
grid on
hold on

a=max(get(gca,'xlim'));
set(gca,'xlim',[0 a]);
```

```

set(gca,'ylim',[0 a]);
line([0 a],[0 a],'color','r')

xlabel('Buff R. sed. exp. Carbon, mg','fontsize',15)
ylabel('Buff R. sed. meas. Carbon, mg','fontsize',15)

error=errperf(mgC_buff_t,mgC_buff,'rmspe');

text(a*.5,a*.2,['RMSE%=' num2str(error,2)],'fontsize',17)

title(['NIST Buffalo River Sediment Stds., ' cruise ' cruise'],...
'fontsize',15)

subplot(2,1,2)

plot(mgC_ace_t,mgC_ace,'o')
grid on
hold on

a=max(get(gca,'xlim'));
set(gca,'xlim',[0 a]);
set(gca,'ylim',[0 a]);
line([0 a],[0 a],'color','r')

xlabel('Acetanilide Chk Stds.,exp. Carbon, mg','fontsize',15)
ylabel('Acetanilide Chk Stds., meas. Carbon, mg','fontsize',15)

error=errperf(mgC_ace_t,mgC_ace,'rmspe');

text(a*.5,a*.2,['RMSE%=' num2str(error,2)],'fontsize',17)

title(['Acetanilide Chk Stds., ' cruise ' cruise'],...
'fontsize',15)
hold off

```

